ELSEVIER

Chemical Physics 204 (1996) 479–483

Chemical Physics

Author index to volume 204

Aamouche, A., G. Berthier, C. Coulombeau, J.P. Flament, M. Ghomi, C. Henriet, H. Jobic and P.Y. Turpin, Molecular force fields of uracil and thymine, through neutron inelastic scattering experiments and scaled quantum mechanical calculations 204 (1996) 353
Ahumada, W., see Cuadros, F. 204 (1996) 41
Alagona, G. and C. Ghio, The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine 204 (1996) 239
Angeli, C. and M. Persico, Quasi-diabatic and adiabatic states and potential energy curves for Na–Cd collisions and excimer formation 204 (1996) 57
Ankerhold, J. and H. Grabert, Quantum effects in barrier dynamics 204 (1996) 27
Aullo, J.M., see Diaz, W. 204 (1996) 195

Bakalarski, G., P. Grochowski, J.S. Kwiatkowski, B. Lesyng and J. Leszczyński, Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory 204 (1996) 301
Balakrishnan, N. and G.D. Billing, Semiclassical wave packet study of V–V energy transfer in highly vibrationally excited CO molecules 204 (1996) 77
Balasubramanian, K., see Kaufman, J.J. 204 (1996) 233
Baňacký, P., see Szőcs, V. 204 (1996) 15
Berthier, G., see Aamouche, A. 204 (1996) 353
Bertrán, J., see Camanyes, S. 204 (1996) 419
Bhaumik, S.R., A. Saran and G. Govil, PCILO investigations on the conformation of two-base hairpin loop in DNA 204 (1996) 205
Billing, G.D., see Balakrishnan, N. 204 (1996) 77
Brańka, A.C., P. Pierański and K.W. Wojciechowski, Confined planar mesoscopic suspensions in external field: Brownian dynamics simulations 204 (1996) 51
Brinck, T., see Murray, J.S. 204 (1996) 289
Broch, H., see Hamza, A. 204 (1996) 373
Brooke-Taylor, C.A., G.H. Grant, A.H. Elcock and W.G. Richards, Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics 204 (1996) 251

Cacelli, I. and V. Carravetta, Calculation of the differential photoionization cross section of HF 204 (1996) 89
Camanyes, S., J.M. Lluch and J. Bertrán, On the deprotonation of the cation radicals of substituted ethylenes. A heterolytic or homolytic process? 204 (1996) 419
Canters, G.W., see Farver, O. 204 (1996) 271
Carravetta, V., see Cacelli, I. 204 (1996) 89
Cedillo, A., see Chattaraj, P.K. 204 (1996) 429

Chaquin, P., see Pettersen, M.V. 204 (1996) 115
Chattaraj, P.K., A. Cedillo and R.G. Parr, Chemical softness in model electronic systems: dependence on temperature and chemical potential 204 (1996) 429
Cieplak, P., see Pohorille, A. 204 (1996) 337
Coitiño, E.L. and J. Tomasi, Solvent effects on the internal rotation of neutral and protonated glyoxal 204 (1996) 391
Coulombeau, C., see Aamouche, A. 204 (1996) 353
Cuadros, F., W. Ahumada and A. Mulero, The high temperature approximation and linearity of the thermodynamic properties on the WCA perturbation parameter 204 (1996) 41

Del Re, G., see Peluso, A. 204 (1996) 347
De Vries, A.H., see Zijlstra, R.W.J. 204 (1996) 439
Diaz, W., J.M. Aullo, M. Paulino and O. Tapia, Transition structure and reactive complexes for hydride transfer in an isoalloxazine–nicotinamide complex. On the catalytic mechanism of glutathione reductase. An ab initio MO SCF study 204 (1996) 195

Elcock, A.H., see Brooke-Taylor, C.A. 204 (1996) 251

Farver, O., L.K. Skov, G. Gilardi, G. van Pouderoyen, G.W. Canters, S. Wherland and I. Pecht, Structure-function correlation of intramolecular electron transfer in wild type and single-site mutated azurins 204 (1996) 271
Felder, P., see Thelen, M.-A. 204 (1996) 135
Fercu, D., see Klopman, G. 204 (1996) 181
Flament, J.P., see Aamouche, A. 204 (1996) 353
Fukui, K., see Nakai, S. 204 (1996) 313
Fülscher, M.P. and E.L. Mehler, The effect of hydrogen bonding on protonation energies and ion pair formation 204 (1996) 403
Furlan, M., see Miertus, S. 204 (1996) 173

Garzillo, C., see Peluso, A. 204 (1996) 347
Ghio, C., see Alagona, G. 204 (1996) 239
Ghomi, M., see Aamouche, A. 204 (1996) 353
Gilardi, G., see Farver, O. 204 (1996) 271
Govil, G., see Bhaumik, S.R. 204 (1996) 205
Grabert, H., see Ankerhold, J. 204 (1996) 27
Grant, G.H., see Brooke-Taylor, C.A. 204 (1996) 251
Grimme, S. and S.D. Peyerimhoff, Theoretical study of the structures and racemization barriers of [*n*]helicenes ($n = 3$–6, 8) 204 (1996) 411
Grochowski, P., see Bakalarski, G. 204 (1996) 301
Guilbert, C., F. Pecorari, D. Perahia and L. Mouawad, Low frequency motions in phosphoglycerate kinase. A normal mode analysis 204 (1996) 327

Hamza, A., H. Broch and D. Vasilescu, Quantum molecular study of S-methylated forms of sulfur mustard 204 (1996) 373
Henriet, C., see Aamouche, A. 204 (1996) 353
Hobza, P., see Šponer, J. 204 (1996) 365

Hoffmann, R., see Vajenine, G.V. 204 (1996) 469
Hormes, J., see Wollersheim, O. 204 (1996) 129

Jacob, J., see Klopman, G. 204 (1996) 181
Jobic, H., see Aamouche, A. 204 (1996) 353
Jóhannesson, G.H., see Kvaran, Á. 204 (1996) 65

Kaufman, J.J., W.S. Koski, S. Roszak and K. Balasubramanian, Correlation between energetics and toxicities of single-carbon halides 204 (1996) 233
Keller, D.A., see Marcus, E. 204 (1996) 157
Klopman, G., D. Fercu and J. Jacob, Computer-aided study of the relationship between structure and antituberculosis activity of a series of isoniazid derivatives 204 (1996) 181
Koski, W.S., see Kaufman, J.J. 204 (1996) 233
Kühn, O., T. Renger and V. May, Theory of exciton–vibrational dynamics in molecular dimers 204 (1996) 99
Kvaran, Á., G.H. Jóhannesson and H. Wang, Rotational perturbations in the (2 + 1) REMPI spectrum of the Rydberg state $[^2\Pi_{3/2}]_c 5d;1g$ of I_2 204 (1996) 65
Kwiatkowski, J.S., see Bakalarski, G. 204 (1996) 301

Lasson, E., see Pettersen, M.V. 204 (1996) 115
Lavery, R., see Zakrzewska, K. 204 (1996) 263
Lesyng, B., see Bakalarski, G. 204 (1996) 301
Leszczyński, J., see Bakalarski, G. 204 (1996) 301
Li, X. and J. Paldus, Valence bond description of spin properties of π-conjugated systems 204 (1996) 447
Lluch, J.M., see Camanyes, S. 204 (1996) 419

Madami, A., see Zakrzewska, K. 204 (1996) 263
Manchester, J.I., M.D. Paulsen, R. Rein and R.L. Ornstein, 1,1,1-Trichloroethane-bound cytochrome P450cam dynamics. Does active site water make a difference? 204 (1996) 223
Marcus, E., D.A. Keller, M. Shibata, R.L. Ornstein and R. Rein, Comparing theoretical and experimental backbone-dependent sidechain conformational preferences for linear, branched, aromatic and polar residues 204 (1996) 157
Mariani, M., N.D. Sharp and S.H. Walmsley, The method of homogeneous deformations and many body potentials in crystals 204 (1996) 1
May, V., see Kühn, O. 204 (1996) 99
McWeeny, R., Ionization and attachment in valence bond theory 204 (1996) 463
Mehler, E.L., see Fülscher, M.P. 204 (1996) 403
Miertus, S., M. Furlan, A. Tossi and D. Romeo, Design of new inhibitors of HIV-1 aspartic protease 204 (1996) 173
Mouawad, L., see Guilbert, C. 204 (1996) 327
Mulero, A., see Cuadros, F. 204 (1996) 41
Murray, J.S., T. Brinck and P. Politzer, Relationships of molecular surface electrostatic potentials to some macroscopic properties 204 (1996) 289

Nakai, S., F. Yoneda, T. Yamabe and K. Fukui, A theoretical study of a model of N-tert-butyl-α-phenylnitrone (PBN) as active oxygen species scavenger 204 (1996) 313

Ojha, R.P., see Saran, A. 204 (1996) 213
Ornstein, R.L., see Manchester, J.I. 204 (1996) 223
Ornstein, R.L., see Marcus, E. 204 (1996) 157

Pack, G.R. and L. Wong, Electrostatic effects on the rates of DNA-catalyzed reactions 204 (1996) 279
Paldus, J., see Li, X. 204 (1996) 447
Parr, R.G., see Chattaraj, P.K. 204 (1996) 429
Paulino, M., see Diaz, W. 204 (1996) 195
Paulsen, M.D., see Manchester, J.I. 204 (1996) 223
Pecht, I., see Farver, O. 204 (1996) 271
Pecorari, F., see Guilbert, C. 204 (1996) 327
Peluso, A., C. Garzillo and G. Del Re, Radiationless decay via ESIPT of the first excited singlet of the hemiporphyrazine 204 (1996) 347
Perahia, D., see Guilbert, C. 204 (1996) 327
Persico, M., see Angeli, C. 204 (1996) 57
Pettersen, M.V., L. Schriver-Mazzuoli, A. Schriver, P. Chaquin and E. Lasson, Reactions of $O(^1D)$ oxygen atom with 1,1,1-trichloroethane in solid argon 204 (1996) 115
Peyerimhoff, S.D., see Grimme, S. 204 (1996) 411
Pierański, P., see Brańka, A.C. 204 (1996) 51
Pohorille, A., P. Cieplak and M.A. Wilson, Interactions of anesthetics with the membrane-water interface 204 (1996) 337
Politzer, P., see Murray, J.S. 204 (1996) 289

Rein, R., see Manchester, J.I. 204 (1996) 223
Rein, R., see Marcus, E. 204 (1996) 157
Renger, T., see Kühn, O. 204 (1996) 99
Richards, W.G., see Brooke-Taylor, C.A. 204 (1996) 251
Romeo, D., see Miertus, S. 204 (1996) 173
Roszak, S., see Kaufman, J.J. 204 (1996) 233

Saran, A. and R.P. Ojha, PCILO studies on anti-AIDS agents: conformation of ddG and ddAPR 204 (1996) 213
Saran, A., see Bhaumik, S.R. 204 (1996) 205
Schmid, W., T. Vogtmann and M. Schwoerer, Influence of two-photon processes on the nonlinear optical response of polydiacetylene single crystals in the near-resonant spectral range 204 (1996) 147
Schriver, A., see Pettersen, M.V. 204 (1996) 115
Schriver-Mazzuoli, L., see Pettersen, M.V. 204 (1996) 115
Schwoerer, M., see Schmid, W. 204 (1996) 147
Sharp, N.D., see Mariani, M. 204 (1996) 1
Shibata, M., see Marcus, E. 204 (1996) 157
Skov, L.K., see Farver, O. 204 (1996) 271
Šponer, J. and P. Hobza, Nonempirical ab initio calculations on DNA base pairs 204 (1996) 365
Szőcs, V. and P. Bañacký, Possibility of a quasiparticle localization at the dissipative dynamics of a nonlinear degenerate adiabatic dimer 204 (1996) 15

Tapia, O., see Diaz, W. 204 (1996) 195
Thelen, M.-A. and P. Felder, Photodissociation of CF_3Br at 193 nm: evidence for a distorted dissociation pathway 204 (1996) 135
Tomasi, J., see Coitiño, E.L. 204 (1996) 391
Tossi, A., see Miertus, S. 204 (1996) 173
Turpin, P.Y., see Aamouche, A. 204 (1996) 353

Vajenine, G.V., R. Hoffmann and H.-C. zur Loye, The electronic structures and magnetic properties of one-dimensional ABO_6 chains in Sr_3ABO_6 (A = Co, Ni; B = Pt, Ir) and two-dimensional MO_3 sheets in $InMO_3$ (M = Fe, Mn) 204 (1996) 469
Van Duijnen, P.Th., see Zijlstra, R.W.J. 204 (1996) 439
Van Pouderoyen, G., see Farver, O. 204 (1996) 271
Vasilescu, D., see Hamza, A. 204 (1996) 373
Vogtmann, T., see Schmid, W. 204 (1996) 147

Walmsley, S.H., see Mariani, M. 204 (1996) 1
Wang, H., see Kvaran, Á. 204 (1996) 65
Wherland, S., see Farver, O. 204 (1996) 271
Wilson, M.A., see Pohorille, A. 204 (1996) 337
Wojciechowski, K.W., see Brańka, A.C. 204 (1996) 51
Wollersheim, O. and J. Hormes, Quantitative in situ FTIR studies of polymers irradiated with synchrotron radiation 204 (1996) 129
Wong, L., see Pack, G.R. 204 (1996) 279

Yamabe, T., see Nakai, S. 204 (1996) 313
Yoneda, F., see Nakai, S. 204 (1996) 313

Zakrzewska, K., A. Madami and R. Lavery, Poisson–Boltzmann calculations for nucleic acids and nucleic acids complexes 204 (1996) 263
Zijlstra, R.W.J., P.Th. van Duijnen and A.H. de Vries, Polarization of the excited states of twisted ethylene in a non-symmetrical environment 204 (1996) 439
zur Loye, H.-C., see Vajenine, G.V. 204 (1996) 469

ELSEVIER

Chemical Physics 204 (1996) 484–494

Chemical Physics

Subject index to volume 204

Methods

Theoretical

Classical mechanics

The method of homogeneous deformations and many body potentials in crystals, M. Mariani, N.D. Sharp and S.H. Walmsley 204 (1996) 1

Many body and quasiparticle approaches

Chemical softness in model electronic systems: dependence on temperature and chemical potential, P.K. Chattaraj, A. Cedillo and R.G. Parr 204 (1996) 429
Valence bond description of spin properties of π-conjugated systems, X. Li and J. Paldus 204 (1996) 447

Transport quantum mechanics

Possibility of a quasiparticle localization at the dissipative dynamics of a nonlinear degenerate adiabatic dimer, V. Szőcs and P. Bańacký 204 (1996) 15
Quantum effects in barrier dynamics, J. Ankerhold and H. Grabert 204 (1996) 27

Equilibrium statistical mechanics

The high temperature approximation and linearity of the thermodynamic properties on the WCA perturbation parameter, F. Cuadros, W. Ahumada and A. Mulero 204 (1996) 41
Confined planar mesoscopic suspensions in external field: Brownian dynamics simulations, A.C. Brańka, P. Pierański and K.W. Wojciechowski 204 (1996) 51
Electrostatic effects on the rates of DNA-catalyzed reactions, G.R. Pack and L. Wong 204 (1996) 279
Chemical softness in model electronic systems: dependence on temperature and chemical potential, P.K. Chattaraj, A. Cedillo and R.G. Parr 204 (1996) 429

Non-equilibrium thermodynamic and hydrodynamic theories

Possibility of a quasiparticle localization at the dissipative dynamics of a nonlinear degenerate adiabatic dimer, V. Szőcs and P. Bańacký 204 (1996) 15

Ab initio schemes for stationary properties

Quasi-diabatic and adiabatic states and potential energy curves for Na–Cd collisions and excimer formation, C. Angeli and M. Persico 204 (1996) 57
Transition structure and reactive complexes for hydride transfer in an isoalloxazine–nicotinamide complex. On the catalytic mechanism of glutathione reductase. An ab initio MO SCF study, W. Diaz, J.M. Aullo, M. Paulino and O. Tapia 204 (1996) 195

Correlation between energetics and toxicities of single-carbon halides, J.J. Kaufman, W.S. Koski, S. Roszak and K. Balasubramanian 204 (1996) 233
Relationships of molecular surface electrostatic potentials to some macroscopic properties, J.S. Murray, T. Brinck and P. Politzer 204 (1996) 289
Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory, G. Bakalarski, P. Grochowski, J.S. Kwiatkowski, B. Lesyng and J. Leszczyński 204 (1996) 301
A theoretical study of a model of N-tert-butyl-α-phenylnitrone (PBN) as active oxygen species scavenger, S. Nakai, F. Yoneda, T. Yamabe and K. Fukui 204 (1996) 313
Solvent effects on the internal rotation of neutral and protonated glyoxal, E.L. Coitiño and J. Tomasi 204 (1996) 391
The effect of hydrogen bonding on protonation energies and ion pair formation, M.P. Fülscher and E.L. Mehler 204 (1996) 403
Theoretical study of the structures and racemization barriers of [*n*]helicenes ($n = 3$–6, 8), S. Grimme and S.D. Peyerimhoff 204 (1996) 411
On the deprotonation of the cation radicals of substituted ethylenes. A heterolytic or homolytic process?, S. Camanyes, J.M. Lluch and J. Bertrán 204 (1996) 419
Polarization of the excited states of twisted ethylene in a non-symmetrical environment, R.W.J. Zijlstra, P.Th. van Duijnen and A.H. de Vries 204 (1996) 439
Ionization and attachment in valence bond theory, R. McWeeny 204 (1996) 463

Computational and simulation methods

Confined planar mesoscopic suspensions in external field: Brownian dynamics simulations, A.C. Brańka, P. Pierański and K.W. Wojciechowski 204 (1996) 51
Rotational perturbations in the (2 + 1) REMPI spectrum of the Rydberg state $[^2\Pi_{3/2}]_c 5d;1g$ of I_2, Á. Kvaran, G.H. Jóhannesson and H. Wang 204 (1996) 65
Comparing theoretical and experimental backbone-dependent sidechain conformational preferences for linear, branched, aromatic and polar residues, E. Marcus, D.A. Keller, M. Shibata, R.L. Ornstein and R. Rein 204 (1996) 157
Design of new inhibitors of HIV-1 aspartic protease, S. Miertus, M. Furlan, A. Tossi and D. Romeo 204 (1996) 173
Computer-aided study of the relationship between structure and antituberculosis activity of a series of isoniazid derivatives, G. Klopman, D. Fercu and J. Jacob 204 (1996) 181
PCILO investigations on the conformation of two-base hairpin loop in DNA, S.R. Bhaumik, A. Saran and G. Govil 204 (1996) 205
PCILO studies on anti-AIDS agents: conformation of ddG and ddAPR, A. Saran and R.P. Ojha 204 (1996) 213
1,1,1-Trichloroethane-bound cytochrome P450cam dynamics. Does active site water make a difference?, J.I. Manchester, M.D. Paulsen, R. Rein and R.L. Ornstein 204 (1996) 223
The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine, G. Alagona and C. Ghio 204 (1996) 239
Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics, C.A. Brooke-Taylor, G.H. Grant, A.H. Elcock and W.G. Richards 204 (1996) 251
Poisson–Boltzmann calculations for nucleic acids and nucleic acids complexes, K. Zakrzewska, A. Madami and R. Lavery 204 (1996) 263
Electrostatic effects on the rates of DNA-catalyzed reactions, G.R. Pack and L. Wong 204 (1996) 279

Low frequency motions in phosphoglycerate kinase. A normal mode analysis, C. Guilbert, F. Pecorari, D. Perahia and L. Mouawad 204 (1996) 327
Interactions of anesthetics with the membrane-water interface, A. Pohorille, P. Cieplak and M.A. Wilson 204 (1996) 337
Radiationless decay via ESIPT of the first excited singlet of the hemiporphyrazine, A. Peluso, C. Garzillo and G. Del Re 204 (1996) 347
Molecular force fields of uracil and thymine, through neutron inelastic scattering experiments and scaled quantum mechanical calculations, A. Aamouche, G. Berthier, C. Coulombeau, J.P. Flament, M. Ghomi, C. Henriet, H. Jobic and P.Y. Turpin 204 (1996) 353
Nonempirical ab initio calculations on DNA base pairs, J. Šponer and P. Hobza 204 (1996) 365
Quantum molecular study of S-methylated forms of sulfur mustard, A. Hamza, H. Broch and D. Vasilescu 204 (1996) 373
Theoretical study of the structures and racemization barriers of [*n*]helicenes ($n = 3$–6, 8), S. Grimme and S.D. Peyerimhoff 204 (1996) 411
Polarization of the excited states of twisted ethylene in a non-symmetrical environment, R.W.J. Zijlstra, P.Th. van Duijnen and A.H. de Vries 204 (1996) 439
The electronic structures and magnetic properties of one-dimensional ABO_6 chains in Sr_3ABO_6 (A = Co, Ni; B = Pt, Ir) and two-dimensional MO_3 sheets in $InMO_3$ (M = Fe, Mn), G.V. Vajenine, R. Hoffmann and H.-C. zur Loye 204 (1996) 469

Molecular dynamics and scattering theory
Semiclassical wave packet study of V–V energy transfer in highly vibrationally excited CO molecules, N. Balakrishnan and G.D. Billing 204 (1996) 77
Theory of exciton–vibrational dynamics in molecular dimers, O. Kühn, T. Renger and V. May 204 (1996) 99

Experimental

Magnetic resonances
PCILO investigations on the conformation of two-base hairpin loop in DNA, S.R. Bhaumik, A. Saran and G. Govil 204 (1996) 205

Infrared spectroscopy
Reactions of $O(^1D)$ oxygen atom with 1,1,1-trichloroethane in solid argon, M.V. Pettersen, L. Schriver-Mazzuoli, A. Schriver, P. Chaquin and E. Lasson 204 (1996) 115
Quantitative in situ FTIR studies of polymers irradiated with synchrotron radiation, O. Wollersheim and J. Hormes 204 (1996) 129

Visible and UV spectroscopy
Valence bond description of spin properties of π-conjugated systems, X. Li and J. Paldus 204 (1996) 447

Laser methods
Photodissociation of CF_3Br at 193 nm: evidence for a distorted dissociation pathway, M.-A. Thelen and P. Felder 204 (1996) 135

Non-linear optical spectroscopy
Influence of two-photon processes on the nonlinear optical response of polydiacetylene single crystals in the near-resonant spectral range, W. Schmid, T. Vogtmann and M. Schwoerer 204 (1996) 147

Multiple resonance spectroscopy
Rotational perturbations in the (2 + 1) REMPI spectrum of the Rydberg state $[^2\Pi_{3/2}]_c$5d;1g of I_2, Á. Kvaran, G.H. Jóhannesson and H. Wang 204 (1996) 65

Atomic and molecular beam techniques
Photodissociation of CF_3Br at 193 nm: evidence for a distorted dissociation pathway, M.-A. Thelen and P. Felder 204 (1996) 135

Time-resolved experiments
Structure-function correlation of intramolecular electron transfer in wild type and single-site mutated azurins, O. Farver, L.K. Skov, G. Gilardi, G. van Pouderoyen, G.W. Canters, S. Wherland and I. Pecht 204 (1996) 271

Mass spectrometry
Photodissociation of CF_3Br at 193 nm: evidence for a distorted dissociation pathway, M.-A. Thelen and P. Felder 204 (1996) 135
Correlation between energetics and toxicities of single-carbon halides, J.J. Kaufman, W.S. Koski, S. Roszak and K. Balasubramanian 204 (1996) 233

Radiolysis
Structure-function correlation of intramolecular electron transfer in wild type and single-site mutated azurins, O. Farver, L.K. Skov, G. Gilardi, G. van Pouderoyen, G.W. Canters, S. Wherland and I. Pecht 204 (1996) 271

Neutron scattering
Molecular force fields of uracil and thymine, through neutron inelastic scattering experiments and scaled quantum mechanical calculations, A. Aamouche, G. Berthier, C. Coulombeau, J.P. Flament, M. Ghomi, C. Henriet, H. Jobic and P.Y. Turpin 204 (1996) 353

Objects

Bulk systems

Gases
The high temperature approximation and linearity of the thermodynamic properties on the WCA perturbation parameter, F. Cuadros, W. Ahumada and A. Mulero 204 (1996) 41
Calculation of the differential photoionization cross section of HF, I. Cacelli and V. Carravetta 204 (1996) 89

Liquids neat
Relationships of molecular surface electrostatic potentials to some macroscopic properties, J.S. Murray, T. Brinck and P. Politzer 204 (1996) 289

Liquid mixtures and solutions
The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine, G. Alagona and C. Ghio 204 (1996) 239

Solvent effects on the internal rotation of neutral and protonated glyoxal, E.L. Coitiño and J. Tomasi 204 (1996) 391

Crystals

The method of homogeneous deformations and many body potentials in crystals, M. Mariani, N.D. Sharp and S.H. Walmsley 204 (1996) 1

Molecular force fields of uracil and thymine, through neutron inelastic scattering experiments and scaled quantum mechanical calculations, A. Aamouche, G. Berthier, C. Coulombeau, J.P. Flament, M. Ghomi, C. Henriet, H. Jobic and P.Y. Turpin 204 (1996) 353

-neat

Relationships of molecular surface electrostatic potentials to some macroscopic properties, J.S. Murray, T. Brinck and P. Politzer 204 (1996) 289

-mixed

Reactions of $O(^1D)$ oxygen atom with 1,1,1-trichloroethane in solid argon, M.V. Pettersen, L. Schriver-Mazzuoli, A. Schriver, P. Chaquin and E. Lasson 204 (1996) 115

Polymers

Quantitative in situ FTIR studies of polymers irradiated with synchrotron radiation, O. Wollersheim and J. Hormes 204 (1996) 129

Influence of two-photon processes on the nonlinear optical response of polydiacetylene single crystals in the near-resonant spectral range, W. Schmid, T. Vogtmann and M. Schwoerer 204 (1996) 147

Surfaces

Interactions of anesthetics with the membrane-water interface, A. Pohorille, P. Cieplak and M.A. Wilson 204 (1996) 337

Low-dimensional materials

Confined planar mesoscopic suspensions in external field: Brownian dynamics simulations, A.C. Brańka, P. Pierański and K.W. Wojciechowski 204 (1996) 51

The electronic structures and magnetic properties of one-dimensional ABO_6 chains in Sr_3ABO_6 (A = Co, Ni; B = Pt, Ir) and two-dimensional MO_3 sheets in $InMO_3$ (M = Fe, Mn), G.V. Vajenine, R. Hoffmann and H.-C. zur Loye 204 (1996) 469

Dielectrics

Polarization of the excited states of twisted ethylene in a non-symmetrical environment, R.W.J. Zijlstra, P.Th. van Duijnen and A.H. de Vries 204 (1996) 439

Biological systems

Computer-aided study of the relationship between structure and antituberculosis activity of a series of isoniazid derivatives, G. Klopman, D. Fercu and J. Jacob 204 (1996) 181

Transition structure and reactive complexes for hydride transfer in an isoalloxazine–nicotinamide complex. On the catalytic mechanism of glutathione reductase. An ab initio MO SCF study, W. Diaz, J.M. Aullo, M. Paulino and O. Tapia 204 (1996) 195

PCILO investigations on the conformation of two-base hairpin loop in DNA, S.R. Bhaumik, A. Saran and G. Govil 204 (1996) 205

PCILO studies on anti-AIDS agents: conformation of ddG and ddAPR, A. Saran and R.P. Ojha 204 (1996) 213
1,1,1-Trichloroethane-bound cytochrome P450cam dynamics. Does active site water make a difference?, J.I. Manchester, M.D. Paulsen, R. Rein and R.L. Ornstein 204 (1996) 223
The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine, G. Alagona and C. Ghio 204 (1996) 239
Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics, C.A. Brooke-Taylor, G.H. Grant, A.H. Elcock and W.G. Richards 204 (1996) 251
Electrostatic effects on the rates of DNA-catalyzed reactions, G.R. Pack and L. Wong 204 (1996) 279
Interactions of anesthetics with the membrane-water interface, A. Pohorille, P. Cieplak and M.A. Wilson 204 (1996) 337

Microscopic systems

Molecules (neutral and ionic)

The high temperature approximation and linearity of the thermodynamic properties on the WCA perturbation parameter, F. Cuadros, W. Ahumada and A. Mulero 204 (1996) 41
Correlation between energetics and toxicities of single-carbon halides, J.J. Kaufman, W.S. Koski, S. Roszak and K. Balasubramanian 204 (1996) 233
The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine, G. Alagona and C. Ghio 204 (1996) 239
Relationships of molecular surface electrostatic potentials to some macroscopic properties, J.S. Murray, T. Brinck and P. Politzer 204 (1996) 289
A theoretical study of a model of N-tert-butyl-α-phenylnitrone (PBN) as active oxygen species scavenger, S. Nakai, F. Yoneda, T. Yamabe and K. Fukui 204 (1996) 313
Quantum molecular study of S-methylated forms of sulfur mustard, A. Hamza, H. Broch and D. Vasilescu 204 (1996) 373
Ionization and attachment in valence bond theory, R. McWeeny 204 (1996) 463

-diatomic

Quasi-diabatic and adiabatic states and potential energy curves for Na–Cd collisions and excimer formation, C. Angeli and M. Persico 204 (1996) 57
Rotational perturbations in the (2 + 1) REMPI spectrum of the Rydberg state $[^2\Pi_{3/2}]_c 5d;1g$ of I_2, Á. Kvaran, G.H. Jóhannesson and H. Wang 204 (1996) 65
Semiclassical wave packet study of V–V energy transfer in highly vibrationally excited CO molecules, N. Balakrishnan and G.D. Billing 204 (1996) 77

-small polyatomics

Calculation of the differential photoionization cross section of HF, I. Cacelli and V. Carravetta 204 (1996) 89
Reactions of $O(^1D)$ oxygen atom with 1,1,1-trichloroethane in solid argon, M.V. Pettersen, L. Schriver-Mazzuoli, A. Schriver, P. Chaquin and E. Lasson 204 (1996) 115
Photodissociation of CF_3Br at 193 nm: evidence for a distorted dissociation pathway, M.-A. Thelen and P. Felder 204 (1996) 135
Solvent effects on the internal rotation of neutral and protonated glyoxal, E.L. Coitiño and J. Tomasi 204 (1996) 391
On the deprotonation of the cation radicals of substituted ethylenes. A heterolytic or homolytic process?, S. Camanyes, J.M. Lluch and J. Bertrán 204 (1996) 419

Polarization of the excited states of twisted ethylene in a non-symmetrical environment, R.W.J. Zijlstra, P.Th. van Duijnen and A.H. de Vries 204 (1996) 439

-aromatics

Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory, G. Bakalarski, P. Grochowski, J.S. Kwiatkowski, B. Lesyng and J. Leszczyński 204 (1996) 301

Theoretical study of the structures and racemization barriers of [*n*]helicenes ($n = 3$–6, 8), S. Grimme and S.D. Peyerimhoff 204 (1996) 411

Ionization and attachment in valence bond theory, R. McWeeny 204 (1996) 463

-other large

Radiationless decay via ESIPT of the first excited singlet of the hemiporphyrazine, A. Peluso, C. Garzillo and G. Del Re 204 (1996) 347

Valence bond description of spin properties of π-conjugated systems, X. Li and J. Paldus 204 (1996) 447

-polymeric and biological

Comparing theoretical and experimental backbone-dependent sidechain conformational preferences for linear, branched, aromatic and polar residues, E. Marcus, D.A. Keller, M. Shibata, R.L. Ornstein and R. Rein 204 (1996) 157

Design of new inhibitors of HIV-1 aspartic protease, S. Miertus, M. Furlan, A. Tossi and D. Romeo 204 (1996) 173

Computer-aided study of the relationship between structure and antituberculosis activity of a series of isoniazid derivatives, G. Klopman, D. Fercu and J. Jacob 204 (1996) 181

Transition structure and reactive complexes for hydride transfer in an isoalloxazine–nicotinamide complex. On the catalytic mechanism of glutathione reductase. An ab initio MO SCF study, W. Diaz, J.M. Aullo, M. Paulino and O. Tapia 204 (1996) 195

1,1,1-Trichloroethane-bound cytochrome P450cam dynamics. Does active site water make a difference?, J.I. Manchester, M.D. Paulsen, R. Rein and R.L. Ornstein 204 (1996) 223

Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics, C.A. Brooke-Taylor, G.H. Grant, A.H. Elcock and W.G. Richards 204 (1996) 251

Structure-function correlation of intramolecular electron transfer in wild type and single-site mutated azurins, O. Farver, L.K. Skov, G. Gilardi, G. van Pouderoyen, G.W. Canters, S. Wherland and I. Pecht 204 (1996) 271

Low frequency motions in phosphoglycerate kinase. A normal mode analysis, C. Guilbert, F. Pecorari, D. Perahia and L. Mouawad 204 (1996) 327

Molecular force fields of uracil and thymine, through neutron inelastic scattering experiments and scaled quantum mechanical calculations, A. Aamouche, G. Berthier, C. Coulombeau, J.P. Flament, M. Ghomi, C. Henriet, H. Jobic and P.Y. Turpin 204 (1996) 353

Molecular aggregates

Theory of exciton–vibrational dynamics in molecular dimers, O. Kühn, T. Renger and V. May 204 (1996) 99

-dimers

Theory of exciton–vibrational dynamics in molecular dimers, O. Kühn, T. Renger and V. May 204 (1996) 99

Nonempirical ab initio calculations on DNA base pairs, J. Šponer and P. Hobza 204 (1996) 365

-van der Waals molecules
Nonempirical ab initio calculations on DNA base pairs, J. Šponer and P. Hobza 204 (1996) 365

-clusters
The effect of hydrogen bonding on protonation energies and ion pair formation, M.P. Fülscher and E.L. Mehler 204 (1996) 403
On the deprotonation of the cation radicals of substituted ethylenes. A heterolytic or homolytic process?, S. Camanyes, J.M. Lluch and J. Bertrán 204 (1996) 419

-complexes
Design of new inhibitors of HIV-1 aspartic protease, S. Miertus, M. Furlan, A. Tossi and D. Romeo 204 (1996) 173
Poisson–Boltzmann calculations for nucleic acids and nucleic acids complexes, K. Zakrzewska, A. Madami and R. Lavery 204 (1996) 263
The effect of hydrogen bonding on protonation energies and ion pair formation, M.P. Fülscher and E.L. Mehler 204 (1996) 403

Free radicals (including hydronium and muonium)
Correlation between energetics and toxicities of single-carbon halides, J.J. Kaufman, W.S. Koski, S. Roszak and K. Balasubramanian 204 (1996) 233
On the deprotonation of the cation radicals of substituted ethylenes. A heterolytic or homolytic process?, S. Camanyes, J.M. Lluch and J. Bertrán 204 (1996) 419
Valence bond description of spin properties of π-conjugated systems, X. Li and J. Paldus 204 (1996) 447

Phenomena

Molecular structure
Comparing theoretical and experimental backbone-dependent sidechain conformational preferences for linear, branched, aromatic and polar residues, E. Marcus, D.A. Keller, M. Shibata, R.L. Ornstein and R. Rein 204 (1996) 157
Design of new inhibitors of HIV-1 aspartic protease, S. Miertus, M. Furlan, A. Tossi and D. Romeo 204 (1996) 173
Computer-aided study of the relationship between structure and antituberculosis activity of a series of isoniazid derivatives, G. Klopman, D. Fercu and J. Jacob 204 (1996) 181
PCILO investigations on the conformation of two-base hairpin loop in DNA, S.R. Bhaumik, A. Saran and G. Govil 204 (1996) 205
PCILO studies on anti-AIDS agents: conformation of ddG and ddAPR, A. Saran and R.P. Ojha 204 (1996) 213
1,1,1-Trichloroethane-bound cytochrome P450cam dynamics. Does active site water make a difference?, J.I. Manchester, M.D. Paulsen, R. Rein and R.L. Ornstein 204 (1996) 223
The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine, G. Alagona and C. Ghio 204 (1996) 239
Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory, G. Bakalarski, P. Grochowski, J.S. Kwiatkowski, B. Lesyng and J. Leszczyński 204 (1996) 301

A theoretical study of a model of N-tert-butyl-α-phenylnitrone (PBN) as active oxygen species scavenger, S. Nakai, F. Yoneda, T. Yamabe and K. Fukui 204 (1996) 313
The effect of hydrogen bonding on protonation energies and ion pair formation, M.P. Fülscher and E.L. Mehler 204 (1996) 403
Theoretical study of the structures and racemization barriers of [n]helicenes (n = 3–6, 8), S. Grimme and S.D. Peyerimhoff 204 (1996) 411
Polarization of the excited states of twisted ethylene in a non-symmetrical environment, R.W.J. Zijlstra, P.Th. van Duijnen and A.H. de Vries 204 (1996) 439

Vibrations and rotations of molecules
Rotational perturbations in the (2 + 1) REMPI spectrum of the Rydberg state $[^2\Pi_{3/2}]_c 5d;1g$ of I_2, Á. Kvaran, G.H. Jóhannesson and H. Wang 204 (1996) 65
Molecular force fields of uracil and thymine, through neutron inelastic scattering experiments and scaled quantum mechanical calculations, A. Aamouche, G. Berthier, C. Coulombeau, J.P. Flament, M. Ghomi, C. Henriet, H. Jobic and P.Y. Turpin 204 (1996) 353
Solvent effects on the internal rotation of neutral and protonated glyoxal, E.L. Coitiño and J. Tomasi 204 (1996) 391

Electronic structure and states
Quasi-diabatic and adiabatic states and potential energy curves for Na–Cd collisions and excimer formation, C. Angeli and M. Persico 204 (1996) 57
Chemical softness in model electronic systems: dependence on temperature and chemical potential, P.K. Chattaraj, A. Cedillo and R.G. Parr 204 (1996) 429
Valence bond description of spin properties of π-conjugated systems, X. Li and J. Paldus 204 (1996) 447
Ionization and attachment in valence bond theory, R. McWeeny 204 (1996) 463
The electronic structures and magnetic properties of one-dimensional ABO_6 chains in Sr_3ABO_6 (A = Co, Ni; B = Pt, Ir) and two-dimensional MO_3 sheets in $InMO_3$ (M = Fe, Mn), G.V. Vajenine, R. Hoffmann and H.-C. zur Loye 204 (1996) 469

Electric and magnetic properties
Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory, G. Bakalarski, P. Grochowski, J.S. Kwiatkowski, B. Lesyng and J. Leszczyński 204 (1996) 301
The electronic structures and magnetic properties of one-dimensional ABO_6 chains in Sr_3ABO_6 (A = Co, Ni; B = Pt, Ir) and two-dimensional MO_3 sheets in $InMO_3$ (M = Fe, Mn), G.V. Vajenine, R. Hoffmann and H.-C. zur Loye 204 (1996) 469

Molecular interactions
Design of new inhibitors of HIV-1 aspartic protease, S. Miertus, M. Furlan, A. Tossi and D. Romeo 204 (1996) 173
Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics, C.A. Brooke-Taylor, G.H. Grant, A.H. Elcock and W.G. Richards 204 (1996) 251
Electrostatic effects on the rates of DNA-catalyzed reactions, G.R. Pack and L. Wong 204 (1996) 279
Relationships of molecular surface electrostatic potentials to some macroscopic properties, J.S. Murray, T. Brinck and P. Politzer 204 (1996) 289
Interactions of anesthetics with the membrane-water interface, A. Pohorille, P. Cieplak and M.A. Wilson 204 (1996) 337

Nonempirical ab initio calculations on DNA base pairs, J. Šponer and P. Hobza 204 (1996) 365
The effect of hydrogen bonding on protonation energies and ion pair formation, M.P. Fülscher and E.L. Mehler 204 (1996) 403

Coupling of electronic and nuclear motion
Quasi-diabatic and adiabatic states and potential energy curves for Na–Cd collisions and excimer formation, C. Angeli and M. Persico 204 (1996) 57
Theory of exciton–vibrational dynamics in molecular dimers, O. Kühn, T. Renger and V. May 204 (1996) 99

Energy transfer processes
Possibility of a quasiparticle localization at the dissipative dynamics of a nonlinear degenerate adiabatic dimer, V. Szőcs and P. Bařnacký 204 (1996) 15
Semiclassical wave packet study of V–V energy transfer in highly vibrationally excited CO molecules, N. Balakrishnan and G.D. Billing 204 (1996) 77

Intramolecular dynamics
Rotational perturbations in the (2 + 1) REMPI spectrum of the Rydberg state $[^2\Pi_{3/2}]_c 5d;1g$ of I_2, Á. Kvaran, G.H. Jóhannesson and H. Wang 204 (1996) 65
Low frequency motions in phosphoglycerate kinase. A normal mode analysis, C. Guilbert, F. Pecorari, D. Perahia and L. Mouawad 204 (1996) 327

-radiationless transitions
Radiationless decay via ESIPT of the first excited singlet of the hemiporphyrazine, A. Peluso, C. Garzillo and G. Del Re 204 (1996) 347

Coherence loss processes
Possibility of a quasiparticle localization at the dissipative dynamics of a nonlinear degenerate adiabatic dimer, V. Szőcs and P. Bařnacký 204 (1996) 15

Non-linear responses (including optical)
Possibility of a quasiparticle localization at the dissipative dynamics of a nonlinear degenerate adiabatic dimer, V. Szőcs and P. Bařnacký 204 (1996) 15
Influence of two-photon processes on the nonlinear optical response of polydiacetylene single crystals in the near-resonant spectral range, W. Schmid, T. Vogtmann and M. Schwoerer 204 (1996) 147

Reactions (including dissociation)
Quantum effects in barrier dynamics, J. Ankerhold and H. Grabert 204 (1996) 27
A theoretical study of a model of N-tert-butyl-α-phenylnitrone (PBN) as active oxygen species scavenger, S. Nakai, F. Yoneda, T. Yamabe and K. Fukui 204 (1996) 313
Theoretical study of the structures and racemization barriers of [*n*]helicenes (*n* = 3–6, 8), S. Grimme and S.D. Peyerimhoff 204 (1996) 411

-gas phase
Correlation between energetics and toxicities of single-carbon halides, J.J. Kaufman, W.S. Koski, S. Roszak and K. Balasubramanian 204 (1996) 233
On the deprotonation of the cation radicals of substituted ethylenes. A heterolytic or homolytic process?, S. Camanyes, J.M. Lluch and J. Bertrán 204 (1996) 419

-photochemical
Reactions of O(^{1}D) oxygen atom with 1,1,1-trichloroethane in solid argon, M.V. Pettersen, L. Schriver-Mazzuoli, A. Schriver, P. Chaquin and E. Lasson 204 (1996) 115
Photodissociation of CF_3Br at 193 nm: evidence for a distorted dissociation pathway, M.-A. Thelen and P. Felder 204 (1996) 135

Tunnelling
Structure-function correlation of intramolecular electron transfer in wild type and single-site mutated azurins, O. Farver, L.K. Skov, G. Gilardi, G. van Pouderoyen, G.W. Canters, S. Wherland and I. Pecht 204 (1996) 271

Electron transfer
Transition structure and reactive complexes for hydride transfer in an isoalloxazine–nicotinamide complex. On the catalytic mechanism of glutathione reductase. An ab initio MO SCF study, W. Diaz, J.M. Aullo, M. Paulino and O. Tapia 204 (1996) 195
Structure-function correlation of intramolecular electron transfer in wild type and single-site mutated azurins, O. Farver, L.K. Skov, G. Gilardi, G. van Pouderoyen, G.W. Canters, S. Wherland and I. Pecht 204 (1996) 271
Ionization and attachment in valence bond theory, R. McWeeny 204 (1996) 463

Ionization (including Rydberg states)
Calculation of the differential photoionization cross section of HF, I. Cacelli and V. Carravetta 204 (1996) 89

Molecular motion (including diffusive)
1,1,1-Trichloroethane-bound cytochrome P450cam dynamics. Does active site water make a difference?, J.I. Manchester, M.D. Paulsen, R. Rein and R.L. Ornstein 204 (1996) 223
Low frequency motions in phosphoglycerate kinase. A normal mode analysis, C. Guilbert, F. Pecorari, D. Perahia and L. Mouawad 204 (1996) 327

Surface effects and catalysis
Electrostatic effects on the rates of DNA-catalyzed reactions, G.R. Pack and L. Wong 204 (1996) 279

Thermodynamic and transport properties
The high temperature approximation and linearity of the thermodynamic properties on the WCA perturbation parameter, F. Cuadros, W. Ahumada and A. Mulero 204 (1996) 41
Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics, C.A. Brooke-Taylor, G.H. Grant, A.H. Elcock and W.G. Richards 204 (1996) 251

Structure of solids and liquids
Confined planar mesoscopic suspensions in external field: Brownian dynamics simulations, A.C. Brańka, P. Pierański and K.W. Wojciechowski 204 (1996) 51